An Investigation of Rupture in Thin Fluid Films

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Abstract

The behavior of a fluid with a thin capillary meniscus can be modelled by the thin film equation $h_t = -(h^n h_{xxx})_x$ with boundary conditions $h_x = \pm\alpha$ and $h_{xxx} = 0$. In general this problem is not tractable to attempts to find an explicit solution; we are concerned primarily with whether or not the film *ruptures*, that is, if $h(x,t) = 0$ for any x, t. We approach this problem with numerical simulation and refinement analysis, as well as by the examination of energies of the film, e.g. mass, surface area, and coating energy. Other related quantities which are less physical and more abstract are also of interest.

We present a brief analysis of the behavior of some of these energies, as well as a proof that, given certain assumptions, rupture cannot occur in a thin capillary meniscus for $n > 4$. We also present some preliminary discussion of the numerical analysis of the problem.

Contents

Acknowledgments

This document and the associated numerical code were created as part of a Harvey Mudd College Mathematics Department senior thesis project in 2005–2006.

I promised Benj Azose and Lori Thomas I'd attempt to name a theorem or lemma after each of them. This fact is reflected in Chapter 2.

Numerous people deserve credit for keeping me sane ... or at least for not letting me get more insane.

Chapter 1

Introduction

1.1 Preliminaries

1.1.1 The Thin Film Equation

When sheets of fluid are thin enough, their behavior is primarily driven by their surface tension and molecular interactions rather than by bulk matter transport (convection). This behavior can then be modelled by a fourth-order nonlinear degenerate diffusion equation, namely

$$h_t = -\nabla \cdot (f(h)\nabla\Delta h) \tag{1.1}$$

with $f(h) \approx h^n$ as $h \to 0$, which in the one-dimensional case with $f(h)$ exactly equal to h^n becomes

$$h_t = -(h^n h_{xxx})_x. \tag{1.2}$$

Different values of this exponent correspond to different physical conditions. When I am sure what these are, I will include them.

Physical Derivation

I would at some point to include here a physical derivation of the thin film equation, but I don't yet know it.

1.1.2 Terms and Definitions

We say that the film has *ruptured* if $h(x,t) = 0$ for any x, t. Ruptures may be either finite-time or infinite-time.

1.2 The Problems

1.2.1 Boundary Conditions and Initial Conditions

Consider a bounded domain $\Omega = [-L, L]$. The thin film equation is fourth-order in the spatial variable and first-order in the temporal variable, so in order for the thin film equation to be well-posed on this domain, we must specify two boundary conditions at each endpoint $x = \pm L$ and we must also specify the initial position $h(x, 0) = f(x)$.

It is common, for instance, to impose periodic boundary conditions on the film so that any boundary terms resulting from integration by parts are irrelevant.

It is also common to consider a spreading-droplet solution, for which $h(x, t) = 0$ at the boundary and for which h can actually be expressed as a function of t multiplied by a function of a single similarity variable.

We might also fix the height of the film at the boundary and consider pressure boundary conditions, for which $h_{xx}(\pm L) = p$, which is equivalent to a constant external pressure, or current boundary conditions, for which $h_{xxx}(\pm L) = \pm c$, which describes liquid draining out of a region at a constant rate. Both of these types of boundary conditions are treated briefly in Bertozzi (1996).

1.2.2 Positivity

We are concerned with solutions of the thin film equation for which $h(x, t) \geq 0$ for all x, t. The positivity (or non-negativity) of solutions is discussed extensively in Bertozzi (1998).

1.2.3 Rupture

Of primary concern in the study of the thin film equation is the investigation of the film's singularities. We are particularly concerned about this investigation for two reasons. First, the physical applications of microfluidics, e.g. lubrication theory, often depend on the film remaining intact throughout some process, e.g. the application of a UV-protectant film to a pair of sunglasses. Second, there is the practical matter that this is one of the simpler characteristics of the film's behavior for us to investigate while still hoping for some sort of meaningful result.

1.2.4 Numerics

We often use numerical analysis to investigate and model the behavior of these thin films. Frequently, it is possible to motivate a line of theoretical investigation with the output from a numerical simulation, or to compare a theoretical result for a certain situation with the numerical model and check for discrepancies.

1.3 Prior Research

Although this particular branch of fluid dynamics is relatively young, there is already a significant body of work describing results related to the thin film equation itself or to thin-film-type equations generally.

1.3.1 Prior Theoretical Results

A good first summary of the main results in lubrication theory is Bertozzi (1998), which presents an overview of the nature of thin films and discusses in depth the problem of contact lines and interfaces which is ultimately the motivating factor behind this thesis. It also illustrates some of the more familiar recent results and methods, such as characterization of some types of finite-time singularities. Finally, it contains a summary of energy arguments (see Sec. 2.2) for the impossibility of singularities, including an extended discussion on the possibility that there is a specific critical exponent above which the film cannot rupture and that it is unclear whether or not such an exponent would depend on the boundary conditions of the film.

Not all of the theoretical results in lubrication theory directly concern the thin film equation, but even when they do not, their methods may be helpful to us. For instance, King (1993) describes *exact* solutions to the porous medium equation $h_t = \nabla \cdot (h^n \nabla h)$, which is another nonlinear degenerate diffusion equation. Since it generally seems impossible to find exact solutions to the thin film equation, the fact that it *is* possible to find solutions for such a similar equation is of some interest. Furthermore, these equations are shown to be polynomials in the spatial coordinate, much like the polynomials described in Sec. 2.3.

The porous medium equation can also serve as a template for methods of investigating the thin film equation, as in Carrillo and Toscani (2002), in which the authors use techniques from the study of the porous medium equation to show that spreading-droplet solutions of the thin film equation with $n = 1$ decay to the unique strong source-type solution of equivalent mass.

In further results relating to source-type solutions of the thin film equation, Bernoff and Witelski (2002) discusses source-type solutions for $0 < n < 3$ in terms of similarity variables and proves that these solutions are stable. This paper also gives the eigenvalue spectrum and associated eigenfunctions for the $n = 1$ case using the fact that the similarity equation has an exact polynomial solution.

It is also sometimes profitable to examine self-similar singularities of the film, as in Bertozzi (1996), in which power series are used to investigate the behavior of similarity solutions both for the thin film equation and for the modified thin film equation $h_t + h^n h_{xxxx} = 0$. This paper also presents results concerning the values of the exponent n for which the modified equation experiences a finite-time singularity and for which they experience infinite-time singularity. This question is of some interest to us in the study of the unmodified equation, but as yet no significant results are forthcoming.

In the category of results most pertinent to our own research, Laugesen (2004) describes integrals of the form $\int h^p h_x^2 dx$ and shows that they are dissipated for certain values of p and n; that is, that their time derivatives are nonpositive for all t. Further discussion of integrals similar to this and their behavior follows in Sec. 2.2. Laugesen also shows that rupture of the film is impossible for certain values of n; this proof follows in Sec. 1.4.

1.3.2 Prior Numerical Results

In Bertozzi (1998), a numerical scheme is presented for solving the thin film equation; this and similar schemes are expanded upon in Zhornitskaya and Bertozzi (2000) and demonstrated to be positivity-preserving. The schemes are also shown to preserve stability and convergence, which is to say that they do not exhibit false rupture of the film but in fact remain close to the true solution. Using these numerical methods, data have been generated that support the hypothesis that rupture may be impossible for $n \geq 2$, but this has not yet been borne out by theory. There are theoretical results, as shown in Bertozzi et al. (1994), that indicate that *if* it can be shown that h_{xx} is bounded for all time, then there can in fact be no rupture for $n \geq 2$, but this boundedness has not been proven.

Bertozzi (1996) also uses numerical schemes to support some of the results achieved in that paper, discussed above in 1.3.1; for instance, simulations are used to compare similarity shape of singularities and the time dependence of the minimum thickness of the film to the theoretical predictions. This is similar to the refinement analysis we will carry out in Sec. 3.3.

1.4 A Prior No-Rupture Proof

Since the determination of whether or not a film ruptures is the problem of primary importance in the study of the thin film equation, it may be worthwhile to reproduce a preexisting characterization of instances in which it is impossible for the film to rupture. The following proof is due to Laugesen (2004), based on earlier work in Bertozzi et al. (1994). I reproduce it here with some additional explanation of the steps involved.

Theorem 1.1. *(Laugesen) Suppose that $h(x,t)$ solves the thin film equation $h_t = -(h^n h_{xxx})_x$ with periodic boundary conditions and $h(x,0) > 0$. Then h cannot experience rupture for $n > 3.5$.*

Proof. Define the quantities $E = \int_\Omega h_x^2\, dx$ and $P_m = \int_\Omega h^m\, dx$. Then by the Cauchy-Schwartz inequality, we know that

$$\begin{aligned} \sqrt{EP_m} &\geq \int_\Omega |h^{m/2} h_x|\, dx \\ &= C\int_\Omega |\frac{\partial}{\partial x} h^{m/2+1}|\, dx, \end{aligned}$$

where $C = 1/|m/2+1|$. We also know that in general, for a periodic function f,

$$\int_\Omega |f_x|\, dx \geq \max(f) - \min(f),$$

so for $f_x = h^{m/2+1}$ we conclude that

$$\sqrt{EP_m} \geq C[\max(h^{m/2+1}) - \min(h^{m/2+1})].$$

Now suppose that $m/2+1 < 0$ and that E and P_m are bounded. Then we know that $\max(h) > \bar{h}$, where $\bar{h}$ is the average value of h, so since $m/2+1 < 0$, we know that $\min(h^{m/2+1}) < \bar{h}^{m/2+1}$, which is constant.

Therefore $C\min(h^{m/2+1}) + \sqrt{EP_m}$ is bounded and thus $\max(h^{m/2+1})$ is bounded since

$$\min(h^{m/2+1}) + \frac{1}{C}\sqrt{EP_m} \geq \max(h^{m/2+1}).$$

If it were the case that $h \to 0$, we would have $h^{m/2+1} \to \infty$ since $m/2 + 1 < 0$. But $h^{m/2+1}$ is bounded, so this cannot be the case. Therefore the film cannot rupture.

As Laugesen points out, prior work in Bertozzi et al. (1994) has shown that $\int h^{q+3/2-n} dx$ is dissipated for $q = 0$. Considering this integral as an instance of P_m with $m = q + 3/2 - n$, once we set $q = 0$ and make use of the fact that $m/2 + 1 < 0$ prevents rupture, basic arithmetic shows that rupture cannot occur for $n > 3.5$.

$\square$

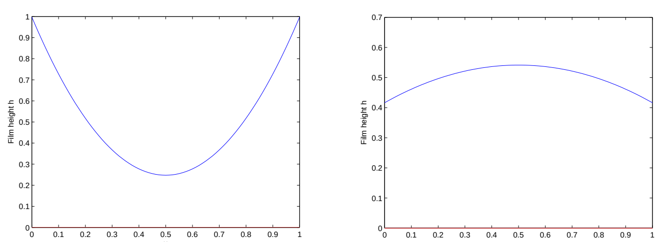
Chapter 2

Theory

2.1 Our Model

We are particularly concerned with the behavior of films which exhibit a thin capillary meniscus; physically, that is, the fluid's adhesion to the walls of its container is not equal to its surface tension.

In relation to the PDE, this means that we consider films over a finite spatial interval $\Omega = [-L, L]$ which have boundary conditions $h_x = \pm\alpha$ and $h_{xxx} = 0$ at $\pm L$. The boundary condition α, by setting the slope of the film, sets the contact angle of the film with the boundary; physically, this value will differ depending on the intrinsic properties of the fluid at hand. The condition $h_{xxx} = 0$ reflects the fact that there is no mass flux at the boundary.



(a) A meniscus with $\alpha = -3$ (b) A meniscus with $\alpha = .5$

Figure 2.1: Examples of thin films for positive and negative contact angles.

Fig. 2.1 shows two pictures of thin films with different contact angles, to illustrate how the choice of α affects the eventual shape of the film.

2.2 Energies

The primary theoretical method for attacking the behavior of the thin film equation is to consider quantities related to the film which we call "energies." Some of these energies have a definite physical relationship with the film, while others need not. The investigation of whether these energies are conserved or dissipated can help us describe the film.

2.2.1 Mass

We define mass as

$$M = \int_\Omega h \, dx.$$

This is not, strictly speaking, the same as the physical expression for mass, as it only captures the volume of the film, which we must multiply by the fluid density ρ in order to get the mass. But in general we assume that the fluid is incompressible and that therefore ρ is constant, so that our definition of mass is within a constant factor of the physical expression.

If our model is to have any hope of approximating a real physical situation, we would want the mass to be conserved; this is in fact the case for our model, and we can present a quick proof.

Theorem 2.1. *For the thin capillary meniscus, mass is conserved.*

Proof. The calculation is straightforward and needs little explanation.

$$\begin{aligned} \frac{\partial}{\partial t} M &= \int_\Omega h_t \, dx \\ &= \int_\Omega -(h^n h_{xxx})_x \, dx \\ &= -h^n h_{xxx}|_{-L}^{L} \\ &= 0, \end{aligned}$$

since $h_{xxx}(\pm L) = 0$. Therefore $\frac{\partial}{\partial t} M = 0$ and thus mass is conserved. □

2.2.2 Surface Area

We define the surface area of the film as

$$A = \int_\Omega h_x^2 \, dx.$$

Again note that this is not the familiar surface area definition from calculus, namely $\int_\Omega \sqrt{1+h_x^2}\,dx$. One of the assumptions built into the thin film equation is that the slope of the film is small ($|h_x| \ll 1$); the fact that this is not always obvious in numerical simulation results is due to rescaling of the equation after this assumption is made.

Since we make the small-slope assumption, we can apply the binomial approximation to the calculus formula for surface area to get

$$\begin{aligned}\int_\Omega \sqrt{1+h_x^2}\,dx &= \int_\Omega 1 + \frac{h_x^2}{2}\,dx \\ &= 2L + \frac{1}{2}\int_\Omega h_x^2\,dx,\end{aligned}$$

so A is a leading-order approximation of the surface area, given the small-slope assumption.

2.2.3 Coating Energy

We are concerned with the behavior of a film exhibiting a thin capillary meniscus. If we consider only mass and surface area, we would expect the film to converge to a flat solution, as this minimizes surface area. Real-world observation indicates, however, that this is clearly not the case. We use coating energy to explain the existence of capillary behavior.

We intuitively define coating energy as a measure of the fluid's "desire" to stick to the walls of the box we put it in. Recalling that $\pm\alpha$ is the slope of the film at $\pm L$, defining the contact angle of the film with the boundary, the coating energy is $\alpha h|_{-L}^{L}$. With the physical intuition that the fluid likes to coat the walls, we suppose that the coating energy decreases the overall energy of the film, so we define an energy in which surface area and coating energy balance each other, as follows:

$$E = \frac{1}{2}\int_\Omega h_x^2\,dx - \alpha h|_{-L}^{L}$$

Theorem 2.2. *For a thin capillary meniscus, E is dissipated.*

Proof. Consider $\frac{\partial}{\partial t}E$ and note that

$$\begin{aligned}\frac{\partial}{\partial t}E &= \frac{\partial}{\partial t}\left[\int_\Omega h_x^2/2\,dx - \alpha h|_{-L}^{L}\right] \\ &= \int_\Omega h_x h_{xt}\,dx - \alpha h_t|_{-L}^{L}\end{aligned}$$

$$= -\int_\Omega h_x(h^n h_{xxx})_{xx}\,dx - \alpha h_t|_{-L}^{L}.$$

Integrating by parts twice, we get

$$\begin{aligned}\frac{\partial}{\partial t}E &= -\int_\Omega \left[h^n h_{xxx}^2 - [h_x(h^n h_{xxx})_x - h_{xx}h^n h_{xxx}]|_{-L}^{L}\right]\,dx - \alpha h_t|_{-L}^{L} \\ &= -\int_\Omega h^n h_{xxx}^2\,dx + h_x h_t|_{-L}^{L} - \alpha h_t|_{-L}^{L} \\ &= -\int_\Omega h^n h_{xxx}^2\,dx\end{aligned}$$

Since $h(x,t) \geq 0$ for all x, t, this integrand is everywhere non-negative, and therefore $\frac{\partial}{\partial t}E \leq 0$, showing that E is dissipated. □

2.3 Minimizers

For energies which are dissipated over time, we would like to know what form the film takes when it has achieved the steady state; that is, how to express the *minimizer* of a particular energy. For some energies this is simple; consider the pure surface energy expression and note that the integral is minimized when $h_x = 0$ for all x, so that assuming surface energy is the only thing driving the film's behavior, the minimizer is a flat film.

However, flat films do not fit our meniscus boundary conditions, in which we generally set the contact angle to be something nonzero. (Nothing prevents us from considering the $\alpha = 0$ case, but it is not particularly interesting or informative.) So we instead consider the coating energy of the film and attempt to find the film that minimizes the energy E, described above in Sec. 2.2.3.

Theorem 2.3. *The minimizer of the energy $E = (1/2)\int_\Omega h_x^2\,dx - \alpha h|_{-L}^{L}$ is a quadratic of the form $\bar{h}(x) = \frac{\alpha x^2}{2L} + b$.*

It is in fact the case that for fixed boundary conditions (and exponents n for which rupture may occur) there is a critical mass above which there is sufficient fluid that the film will not rupture and below which it will. In the following proof I will give a minimizer which is not piecewise defined as quadratics on either side of a central region where $h(x,t) = 0$; we can interpret this as belonging to a film which is above the critical mass and therefore does not rupture (that is, $b > 0$). The proof for a film which is below critical mass corresponds to $b < 0$, for which we actually consider the presence of a dry spot with $h(x,t) = 0$. This is more complicated and will be inserted later.

Proof. Consider the function $\bar{h}(x) = \frac{\alpha x^2}{2L} + b$, where the value of the constant b depends on the mass of the fluid. Then consider a small perturbation δ of the fluid; this perturbation must be massless in order that mass be conserved overall. Also consider E as a function of the perturbation; that is, $E(\delta)$ is the energy of a given film $h = \bar{h} + \delta$, and $E(0)$ is the energy of $\bar{h}$. To show that $\bar{h}$ is a minimizer, it suffices to show that $E(\delta) \geq E(0)$.

$$\begin{aligned}
E(\delta) - E(0) &= \frac{1}{2}\int_\Omega \left[\left(\frac{\alpha x^2}{2L} + b + \delta\right)_x^2 - \left(\frac{\alpha x^2}{2L} + b\right)_x^2 \right] dx \\
&\quad -2\alpha\left(\frac{\alpha L}{2} + b + \delta\right) + 2\alpha\left(\frac{\alpha L}{2} + b\right) \\
&= \frac{1}{2}\int_\Omega \left[\left(\frac{\alpha x}{L} + \delta_x\right)^2 - \left(\frac{\alpha x}{L}\right)^2 \right] dx - 2\alpha\delta \\
&= \frac{1}{2}\int_\Omega \left[\frac{2\alpha x \delta_x}{L} + \delta_x^2 \right] dx - 2\alpha\delta \\
&= \int_\Omega \frac{\delta_x^2}{2}\, dx + \left.\frac{\alpha x \delta}{L}\right|_{-L}^{L} - \int_\Omega \frac{\alpha\delta}{L}\, dx - 2\alpha\delta \\
&= \int_\Omega \frac{\delta_x^2}{2}\, dx,
\end{aligned}$$

since, as we said, δ is massless, so $\int_\Omega (\alpha\delta)/L\, dx = 0$. But $\delta_x^2 \geq 0$, so $E(\delta) - E(0) \geq 0$ and therefore $\bar{h}$ must be a minimizer of the energy E. □

2.4 Boundedness

It is not immediately obvious that the height of the film in a thin capillary meniscus must be bounded, though it is perhaps intuitive. We can prove that the film thickness is, in fact, bounded using energy methods.

Theorem 2.4. *(Benj's Lemma) If $h(x,t)$ solves $h_t = -(h^n h_{xxx})_x$ on $\Omega = [-L, L]$ with $h_x = \pm\alpha$ and $h_{xxx} = 0$ at the boundary, then $h(x,t) < \infty$ for all x, t.*

Proof. Consider the energies

$$E = \int_\Omega h_x^2\, dx - \alpha h|_{-L}^{L} \qquad \text{and} \qquad M = \int_\Omega h\, dx$$

Now consider their product and apply the Cauchy-Schwarz Inequality:

$$\begin{aligned} EM = \int_\Omega h_x^2\,dx \int_\Omega h\,dx - M\alpha h|_{-L}^{L} &\geq \int_\Omega |h_x h^{1/2}|\,dx - M\alpha h|_{-L}^{L} \\ &= \frac{2}{3}\int_\Omega \left|\frac{\partial}{\partial x}h^{3/2}\right|\,dx - M\alpha h|_{-L}^{L} \\ &\geq \frac{2}{3}\max(h^{3/2}) - M\alpha h|_{-L}^{L}, \end{aligned}$$

noting in the last step that $\int_\Omega |f_x|\,dx \geq \max(f) - \min(f)$ for any f and that $\min(h) = 0$.

Then consider that $E(0) > E(t)$ for all t, since E is dissipated. Furthermore, $2M\alpha\,\max(h) \geq M\alpha h|_{-L}^{L}$, so we have the following expression after rearranging the last inequality above:

$$E(0)M + 2M\alpha\,\max(h) \geq \frac{2}{3}\max(h^{3/2}) \tag{2.1}$$

But $h^{3/2}$ dominates h as $h \to \infty$, so since $E(0)M$ is a constant, Eqn. 2.1 is a contradiction if $h \to \infty$. Therefore h must be bounded. □

2.5 No Rupture

Just as Laugesen showed that rupture cannot occur in a film with periodic boundary conditions for $n \geq 3.5$, we can obtain a similar (albeit somewhat weaker) result for the thin capillary meniscus.

Theorem 2.5. *(Thomas Lemma) Assuming that h_{xx} is bounded for all t and that the energy $P_m = \int_\Omega h^m\,dx$ is bounded, there can be no rupture in a thin capillary meniscus for $m < -2$.*

Proof. Consider the thin film equation with capillary meniscus boundary conditions, and consider the energies

$$E = \int_\Omega h_x^2\,dx - \alpha h|_{-L}^{L} \qquad \text{and} \qquad P_m = \int_\Omega h^m\,dx$$

Multiplying these two quantities together and applying the Cauchy-Schwarz inequality, we find that

$$EP_m = \int_\Omega h_x^2\,dx \int_\Omega h^m\,dx - \alpha h|_{-L}^{L} \cdot P_m$$

$$\geq \left(\int_\Omega |h_x h^{m/2}|\,dx\right)^2 - \alpha h|_{-L}^{L} \cdot P_m$$

Now note that $|h_x h^{m/2}| = C\left|\frac{\partial}{\partial x} h^{m/2+1}\right|$, where $C = 1/|1+m/2|$, so

$$EP_m \geq \left(C\int_\Omega \left|\frac{\partial}{\partial x} h^{m/2+1}\right|\,dx\right) - \alpha h|_{-L}^{L} \cdot P_m$$

Furthermore, for all reasonably well-behaved functions f, we know that $\int_\Omega |f_x|\,dx \geq \max(f) - \min(f)$, so

$$EP_m \geq \left(C(\max(h^{m/2+1}) - \min(h^{m/2+1})\right)^2 - \alpha h|_{-L}^{L} \cdot P_m. \qquad (2.2)$$

Now suppose that E and P_m are bounded (see Thm. 2.6), and note that we proved in Theorem 2.4 above that h is bounded, for instance by $\max(h)$.

Using this fact and rearranging terms in Eqn. 2.2, we see that

$$EP_m + 2\alpha\max(h)\cdot P_m \geq \left(C\left[\max(h^{m/2+1}) - \min(h^{m/2+1})\right]\right)^2$$

Since the right-hand side is a perfect square, both sides of this inequality are nonnegative, and therefore we can take square roots of both sides. Also note that E is dissipated, and that therefore $E(0) \geq E(t)$ for all $t > 0$, so we can replace the function E with the constant $E(0)$ while preserving the inequality. Therefore we have

$$\sqrt{(E(0) + 2\alpha\max(h))\cdot P_m} \geq \max(h^{m/2+1}) - \min(h^{m/2+1})$$

Again we can rearrange terms and finally see that

$$\sqrt{(E(0) + 2\alpha\max(h))\cdot P_m} + \min(h^{m/2+1}) \geq \max(h^{m/2+1}).$$

Suppose that $m/2 + 1 < 0$. We know that both terms on the left-hand side of the inequality are bounded, the first term because we supposed all values involved were bounded, the second because

$$\min(h^{m/2+1}) \leq (\max h)^{m/2+1},$$

which is a constant. Therefore $\max(h^{m/2+1})$ is bounded. If it were the case that $h \to 0$ for any x, t, we would have $h^{m/2+1} \to \infty$ since $m/2+1 < 0$. Therefore it cannot be the case that $h \to 0$, and thus a thin capillary meniscus cannot rupture for $m < -2$. □

Note that in the process of this proof we assumed that P_m was bounded. This has not been shown, and in fact P_m is not bounded for certain values of m. We must calculate the values of m for which P_m *is* bounded.

Furthermore, this calculation will allow us to find values of n for which no rupture can occur, which are more valuable to us than values of m for which this is the case, since n is directly involved in the thin film equation itself.

Theorem 2.6. *$P_m = \int_\Omega h^m \, dx$ is dissipated for $2 \le m + n \le 3$, assuming $h_{xx}(L)$ is bounded for all t.*

Proof. Consider $\frac{\partial}{\partial t} P_m$. With copious use of integration by parts, we can carry out the following calculation:

$$\begin{aligned}
\frac{\partial}{\partial t} P_m &= \frac{\partial}{\partial t} \int_\Omega h^m \, dx = \int_\Omega m h^{m-1} h_t \, dx \\
&= -m \int_\Omega h^{m-1} (h^n h_{xxx})_x \, dx \\
&= -m \left[h^{m-1} h^n h_{xxx} |_{-L}^{L} - (m-1) \int_\Omega h^{m-2} h_x h^n h_{xxx} \, dx \right] \\
&= m(m-1) \int_\Omega h^{m+n-2} h_x h_{xxx} \, dx \\
&= m(m-1) \int_\Omega h^{m+n-2} \left[\frac{\partial}{\partial t} (h_x h_{xx}) - h_{xx}^2 \right] \, dx \\
&= -m(m-1) \int_\Omega h^{m+n-2} h_{xx}^2 \, dx + \\
&\quad m(m-1) \left[h^{m+n-2} h_x h_{xx} |_{-L}^{L} - (m+n-2) \int_\Omega h^{m+n-3} h_x^2 h_{xx} \, dx \right] \\
&= m(m-1) h^{m+n-2} h_x h_{xx} |_{-L}^{L} \\
&\quad -m(m-1) \int_\Omega h^{m+n-2} h_{xx}^2 - (m+n-2) h^{m+n-3} h_x^2 h_{xx} \, dx
\end{aligned}$$

Considering the second term (let's call it I) in this integral separately for ease of calculation, we find that

$$\begin{aligned}
I &= \int_\Omega h^{m+n-3} h_x^2 h_{xx} \, dx \\
&= h^{m+n-3} \frac{h_x^3}{3} |_{-L}^{L} - \frac{m+n-3}{3} \int_\Omega h^{m+n-4} h_x^4 \, dx
\end{aligned}$$

So, assuming symmetry, we finally see that

$$\frac{1}{m(m-1)} \frac{\partial}{\partial t} P_m = \int_\Omega -h^{m+n-2} h_{xx}^2 + \frac{(m+n-2)(m+n-3)}{3} h_x^4 \, dx$$

$$+ \quad 2\alpha h^{m+n-2}(L)h_{xx}(L) + 2(m+n-2)\frac{\alpha^3}{3}h^{m+n-3}(L).$$

If we want P_m to be bounded and dissipated, we need the second term in the integral to be negative and we need the boundary terms outside the integral to remain bounded. Therefore we need $h_x x(L)$ to be bounded, which we in fact assumed for the purposes of this proof, and we need $(m+n-2)\cdot(m+n-3) \leq 0$, or $2 \leq m+n \leq 3$ (where $m(m-1) > 0$). □

Now we are ready to state the main result.

Theorem 2.7. *For a thin capillary meniscus with h_{xx} bounded, there can be no rupture for $n > 4$.*

Proof. Given that in Thm. 2.5 we showed that we need $m < -2$ in order to prevent rupture, and that in Thm. 2.6 we showed that we need $2 \leq m+n \leq 3$ in order for the proof of Thm. 2.5 to be valid, we can now find a bound for n above which the film cannot rupture. Since we want the smallest such bound, choose $m+n=2$.

Then since $m+n=2$ and $m < -2$, we can conclude that there can be no rupture in a thin capillary meniscus for $n > 4$. □

Chapter 3

Numerical Analysis

3.1 Implementation

Since exact solutions to the thin film equation are in general difficult to find, we also approach the problem from a numerical standpoint. We chose to use MATLAB for this endeavor in order to make use of its built-in ODE solvers. The original description of this particular implementation is in Bertozzi (1998)

In order to solve the PDE, we first discretize it along the spatial variable into a collection of ODEs. We then input the ODEs as a large system in MATLAB and use a standard ODE solving tool to find a numerical solution. Originally we had been using `ode45`, a generalized Runge-Kutta solver, but the runtime for `ode45` quickly becomes unmanageable for even remotely stiff problems, so we switched to `ode15s`, a solver much better equipped for problems as stiff as this one.

It is worth noting that one primary difference between all our theoretical analysis and this numerical code is that the theoretical analysis has all been done on the interval $[-L, L]$, whereas all numerical computation is normalized to the interval $[0, 1]$.

The MATLAB code for this implementation appears in Appendix A; it is documented there, so we will not reproduce the documentation here.

3.2 Observation of Film Behavior

3.2.1 Rupture and Critical Exponents

Though it has been shown that $n \geq 3.5$ is sufficient to preclude rupture in a film with periodic boundary conditions, and we have shown that $n > 4$ is sufficient for a thin capillary meniscus, it is hypothesized that the actual bound is much lower, and that in fact there may be some critical exponent n_*, possibly dependent on boundary conditions, above which we can definitively state that rupture cannot occur and below which we admit the possibility that rupture may occur. Currently we can guarantee for certain boundary conditions that rupture can occur for $n < 1/2$, but cannot make definitive assertions about $1/2 < n < 7/2$.

Making theoretical progress on this problem is hard, but we can make some numerical observations which seem to bear out this possibility. Consider, for instance, Figure 3.1, in which for $n = 1$ we set the initial condition of the film to be $(.5 - x)^2 + .05e^{-10x^2}$ and allowed the ODE solver to run until the film ruptured. At $t = .00675$, we can see from the figure that the film touches down; after this point the solver cannot continue running because the film height would become negative.

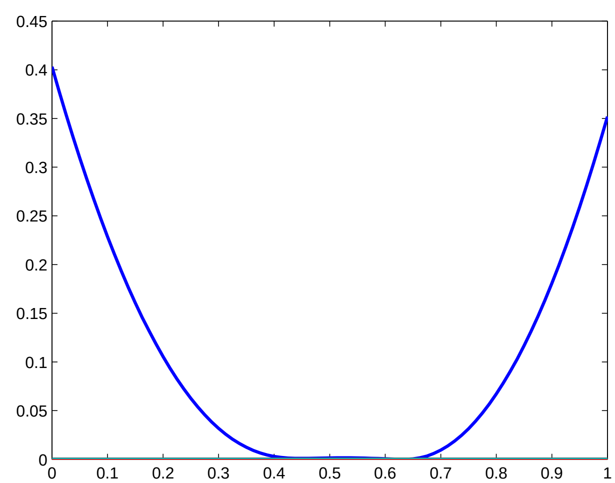


Figure 3.1: A ruptured film with $n = 1$ and $t = .00675$.

Now compare Figure 3.1 to Figure 3.2, which is of a film with the same initial conditions, but with $n = 2$ and the simulation carried out until $t = .15$. The film in Figure 3.2 has not ruptured (though we can see that it is becoming quite thin) despite having been run all the way until $t = .15$, whereas the first film ruptured after only $t = .00675$. Not only that, but this film is beginning to form a droplet in the center, between a pair of points at which the film height is approaching 0, though it has not reached it.

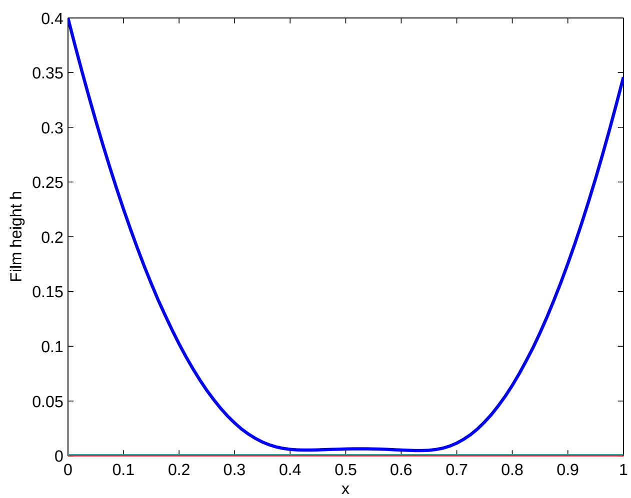


Figure 3.2: A small droplet forming in a film for $n = 2$, $t = .15$.

As we refine the number of gridpoints on which the PDE is being solved, these "squeezing points" may shift position in the interval; certainly their positions shift over time. We can have the MATLAB routine save the data from its simulation and use these data to determine how and how fast these points are shifting, though we have not done any of this yet.

For additional comparison between the rupture and squeeze points for $n = 1$ and $n = 2$, consider the following pair of figures, Figs. 3.3 and 3.4, which zoom in on the right-hand rupture and squeeze points from Figs. 3.1 and 3.2. Note the actual touchdown point in the $n = 1$ case, whereas in the $n = 2$ case a significant film thickness remains.

This comparison of Figs. 3.1 and 3.2 is only one example of many such pairs of figures in which the film is below the critical mass for $n = 1$ and therefore ruptures, yet does not seem to do so in finite time for $n = 2$. It may rupture in infinite time, or it may not rupture at all; it requires further

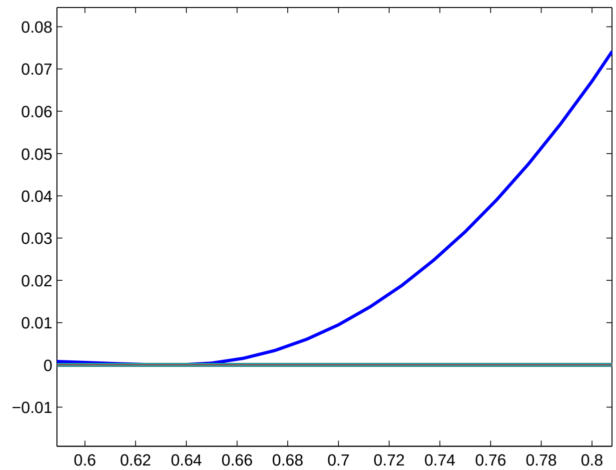


Figure 3.3: A close-up of the rupture in Fig. 3.1 for $n = 1$, $t = .00675$.

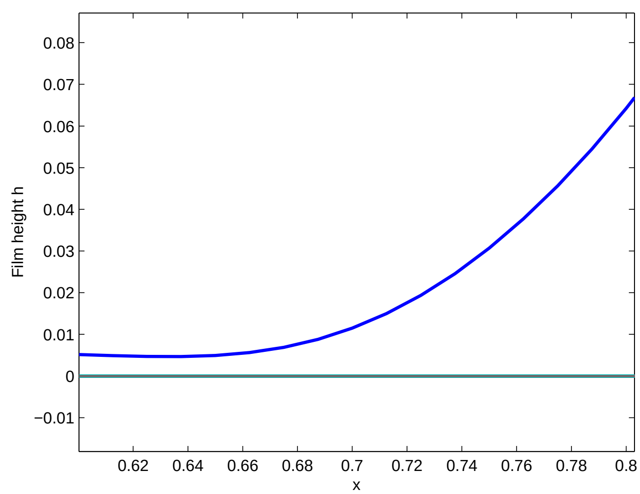


Figure 3.4: A close-up of a squeeze point in Fig. 3.2 for $n = 2$, $t = .15$.

simulation and data analysis to more firmly hypothesize which.

3.2.2 Minimizers

Clearly we would like to know that our theoretical results and the numerical simulations are in agreement. In particular, we would like to know that the numerical code demonstrates that films do in fact approach the quadratic minimizer we gave for the energy E in Sec. 2.2.3.

In practice, however, it is not always obvious that this is the case. Certainly particular initial conditions cause the film to converge quickly to the minimizer, as in Figure 3.5, which had an initial condition of simply the constant .5 across the entire interval and converged to the quadratic minimizer by $t = .05$.

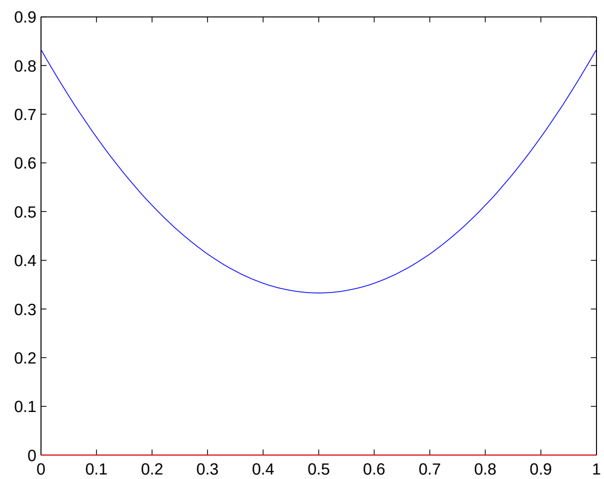


Figure 3.5: Convergence to a minimizer for $n = 2$, $t = .05$.

In other cases, however, such as Figure 3.2 above, rather than achieving the minimizer, the film forms a droplet between two points whose thickness is squeezed as time passes. (In fact, the beginnings of this droplet behavior are often visible in animations of films that *do* achieve their minimizers, but usually the droplet quickly smooths out.) This droplet is not piecewise quadratic, and we would like to know whether the film ever relaxes into a quadratic as current theory suggests it should.

If in fact numerical results continue to suggest that some films do not approach a quadratic minimizer in finite or infinite time, our next goal would be to attempt to prove theoretically that this is can be the case or perhaps find another energy whose minimizers more accurately describe those observed numerically.

3.3 Refinement Analysis

As the film's rupture or failure to rupture are the primary concerns of this research, we supplement our theoretical results with numerical observations using the above implementation of a solver for this PDE. With the data our solver outputs, we can use `minplot.m` (see Appendix A) to generate a plot of the minimum thickness of the film (on a logarithmic scale) against the time t at which these minima occurred. The goal is to use an analysis of these plots of the minima to determine whether or not the film will rupture in finite time, infinite time, or not at all.

The specific method of refinement studies we will use is to halve or double the coarseness of the solution mesh, draw two `minplots` on top of one another, and observe the differences in scaling of film thickness with the coarseness of the mesh.

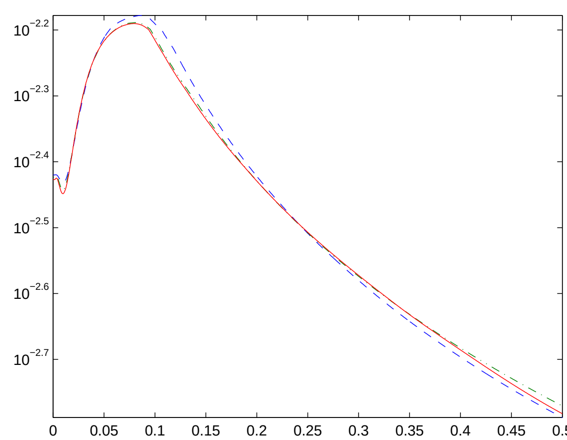


Figure 3.6: Minimimum thickness of the film over time for 40, 80, and 160 gridpoints. The solid line is for 40, the dashed line for 80, and the dotted and dashed line for 160.

As an illustration, consider Figure 3.6, which shows the minimum plots for the same film for which a time snapshot is given in Figure 3.2. The minimum plots are given for 40, 80, and 160 gridpoints; we can already see that the numerical solution is converging fairly well, as these plots lie nearly on top of one another much of the time.

We can also plot the absolute value of the difference between two arrays of values for minimum film thickness over time, usually using the most refined values as a baseline and subtracting the others from these. We could use these plots to see how the error between a well-refined film and an under-refined film is scaling, e.g. proportionally, as the square, and so forth. Figure 3.7 is an example of this type of plot, in which we can see that doubling the number of gridpoints seems to decrease the error in the minimum values of the film by approximately one order of magnitude. The main goal of refinement analysis is to show that the numerical code actually converges to a single solution if the number of gridlines is sufficiently high. From Figs. 3.6 and 3.7, we can see that even at only 160 gridpoints, the code is already converging fairly quickly.

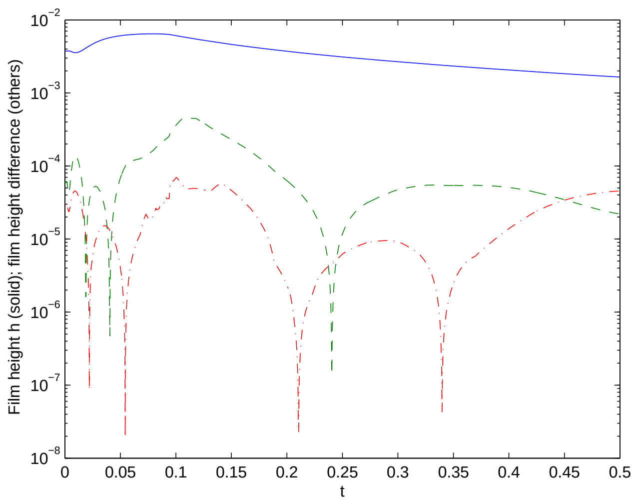


Figure 3.7: Baseline minimum film thickness for 160 gridpoints, with the difference between 160 and 40 as a dashed line and the difference between 160 and 80 as a dotted and dashed line.

In addition to the figures, whose only purpose is to give us a quick visual summary of the behavior of the minimum values, we also save the data which generated these minimum plots so that we can analyze it later.

We can also attempt to track the *location* of these minima. In general, it seems to be the case that the film will do one of the following things:

- Converge to a minimizer without rupture,
- Experience a single touchdown or squeeze point, or
- Experience a pair of touchdown or squeeze points.

In the last case, we wish to observe the change in position of the squeeze points, hoping to determine whether they will move inward and merge together, whether they will stay in one location and simply squeeze progressively thinner, or whether they will disappear and the film will converge to the quadratic minimizer. This is a matter for further investigation. It is also not clear whether it is possible to force the film to experience more than two touchdown points, but so far the numerical simulations generated for this thesis have been unable to do so.

Chapter 4

Future Work

4.1 Theoretical Results

In summary, we have shown that the minimizers of the energy

$$E = \frac{1}{2} \int_{\Omega} h_x^2 \, dx - \alpha h|_{-L}^{L}$$

are piecewise quadratic, proved some dissipation results for the energy $P_m = \int_{\Omega} h^m \, dx$, and proved that there can be no rupture in a thin capillary meniscus for $n > 4$.

There is a relatively large body of theoretical knowledge about the thin film equation for problems other than the thin capillary meniscus. In our continuing work with this problem, one of our primary goals is to formulate and prove results analagous to many of these existing results.

It is also an overarching goal of this thesis to discover or formulate new energies by analysis of which we might be able to further characterize the behavior of the film. For instance, we would like to have a new energy that allows us to lower the bound on the no-rupture proof for the thin capillary meniscus below 4, perhaps to 3.5 as in the case of periodic boundary conditions.

4.2 Numerical Observations

We have illustrated only preliminary work in the numerics of this problem, and there is much still to be done. Much of the remaining numerical work will consist of refinement analysis to various ends, but we will also attempt to compare theoretical results and numerical observations, and it is possible that some new theoretical result we had not yet considered will come out of some numerical insight.

In Sec. 3.3 we saw that for $n = 2$ some films form a solution that, rather than approaching the quadratic minimizer as expected, has two pinching points on either side of a droplet. If in fact the hypothesized critical exponent for the thin film equation exists, and if in fact this exponent is 2 for our boundary conditions (and therefore these films should not rupture), we would like to know if the droplet-forming films ever approach the minimizer at all, and if so whether they do so in finite time or infinite time. It is not clear whether they will achieve the minimizer or whether the film thickness is decreasing fast enough at the pinch points to cut off communication between the droplet and the remainder of the fluid, thereby preventing the film from achieving its minimizer. We may be able to approach this problem with further refinement analysis.

Appendix A

Numerical Code

A.1 System Definitions

In order to numerically solve the thin film equation, we need to discretize it in the spatial variable so that it is accessible to an ODE solver. The file `filmde.m` takes care of defining this system and packaging it in a format that the ODE solver `ode15s` can handle.

```
function systemmat_cols = filmde(t, y)

% FILMDE
% R.M. Baur
% Originally created: 23 Jan 2005
% Last modified: 10 April 2005
% HMC Senior Mathematics Thesis, Spring-Fall 2005

% This is a more streamlined version of earlier code. All
% comments in this file were written on 10 April 2005. Older
% versions of this file are  printed out in my thesis notebook
% and saved in ~/simcode/old-code on my account on the
% mathematics machines.

% FILMDE sets up the system of coupled nonlinear ODEs that
% results from a discretization of the spatial variable of the
% thin film equation. Once this system is set up, it is passed
% to a differential equation solver for evaluation.
```

```
% gridlines (the mesh refinement) and alpha (the contact
% angle at the boundary) are defined in solver.m.

global gridlines alpha

% We need to translate y because the stencil size prevents
% us from calculating y on the two gridpoints at each side of
% the solution space (four incalculable gridlines total) using
% the ODE solver. We will interpolate these values after the
% fact.

for i = 1 : gridlines - 3
    ytrans(i + 2) = y(i);
end

% Here is the necessary interpolation.

ytrans(1) = (12/5)*ytrans(3) - (64/35)*ytrans(4) +  ...
    (3/7)*ytrans(5) - (36/35)*alpha/gridlines;
ytrans(2) = 2*ytrans(3) - (9/7)*ytrans(4) + ...
    (2/7)*ytrans(5) - (2/7)*alpha/gridlines;
ytrans(gridlines) = 2*ytrans(gridlines-1) - ...
    (9/7)*ytrans(gridlines-2) + ...
    (2/7)*ytrans(gridlines-3) - ...
    (2/7)*alpha/gridlines;
ytrans(gridlines+1) = (12/5)*ytrans(gridlines-1) - ...
    (64/35)*ytrans(gridlines-2) + ...
    (3/7)*ytrans(gridlines-3) - ...
    (36/35)*alpha/gridlines;

% Now we set up the difference equations we need in order to
% define the ODE system. These correspond to the difference
% equations in Bertozzi's paper, "The Mathematics of Moving
% Contact Lines in Thin Liquid Films". The b in a difference
% equation's definition indicates a reverse difference
% equation, while the absence of a b indicates a forward
% difference equation.
%
% Note that all limits on the for loops are motivated by our
% ability to calculate the necessary values; some information
```

```
% at the endpoints is necessarily lost each time we calculate
% a set of differences.

for i = 2 : gridlines + 1
    yxb(i) = (ytrans(i) - ytrans(i - 1))*gridlines;
end

for i = 2 : gridlines
    yxx(i) = (yxb(i + 1) - yxb(i))*gridlines;
end

for i = 3 : gridlines
    yxxxb(i) = (yxx(i) - yxx(i - 1))*gridlines;
end

% Now we can finally define the discretized system of ODEs.
% Again note that we cannot define the system all the way
% out to the endpoints; these values will be interpolated
% after solution in solver.m.

for i = 3 : gridlines - 1
    systemmat(i - 2) = ...
        -(a(ytrans(i), ytrans(i + 1))*yxxxb(i + 1) - ...
        a(ytrans(i - 1), ytrans(i))*yxxxb(i))*gridlines;
end

% We output t to give a general idea of how far along we
% are in the solution process. Since ode15s uses a variable
% step size which is, from time to time, negative, this is
% not a completely useful piece of information, but it is
% somewhat helpful.

t

% We defined systemmat above as a row vector; ode15s wants
% a column vector as input. We transpose and then output.

systemmat_cols = transpose(systemmat);
```

A.2 The Function *a*

The function a is is used to define the system of ODEs. It is, in essence, an approximation function of $f(h)$, which in turn for our purposes is generally h^n.

```
function afunc = a(f, g)

% A
% R.M. Baur
% Originally created: 3 February 2005
% Last modified: 10 April 2005
% HMC Mathematics Senior Thesis, Spring-Fall 2005

% This is a more streamlined version of earlier code.
% All comments in this file were written 10 April 2005.
% Older versions of this code are printed out in my thesis
% notebook and saved in ~/simcode/old-code on my account
% on the mathematics machines.

% As given in Bertozzi's paper, "The Mathematics of Moving
% Contact Lines in Thin Liquid Films", the function "a"
% is defined as
% a(s1, s2) = (s1 - s2)/(G'(s1) - G'(s2))
% if s1 \neq s2 and as f(s1) if s1 = s2. Here, f(h) = h^n.
% G, in turn, is defined such that G''(h) = 1/f(h).
% Since f(h) = h^n, G''(h) = 1/h^n, so G'(h) = ln h, -1/h,
% or -1/(2h^2), depending on n (= 1, 2, 3).

% As of this implementation, the user must be aware of
% which value is being used for the exponent in the thin
% film equation and choose the appropriate definition for
% a, commenting out the others.

% USE THIS CODE IF n = 1

if (f ~= g)
   afunc = (f - g)/(log(f) - log(g));
else
```

```
   afunc = f;
end

% USE THIS CODE IF n = 2

% if (f ~= g)
%     afunc = (f - g)/((-1/f) + (1/g));
% else
%     afunc = f^2;
% end

% USE THIS CODE IF n = 3

% if (f ~= g)
%     afunc = (f - g)/((-1/(2*f^2)) + (1/(2*g^2));
% else
%     afunc = f^3;
% end
```

A.3 Numerical Solver

The `solver.m` function takes the system output by `filmde.m` and runs it through the `ode15s` routine. It then uses `deval` to get values of the film height for uniform timesteps (rather than the variable timesteps used by `ode15s`) and plots the values of the film height at each one of these timesteps sequentially, as an animation.

```
function solout = solver;

% SOLVER
% R.M. Baur
% Originally created: 18 February 2005
% Last modified: 10 April 2005
% HMC Senior Mathematics Thesis, Spring-Fall 2005

% This is a more streamlined version of earlier code. All
```

```
% comments in this file were written 10 April 2005. Older
% versions of this file are printed out in my thesis
% notebook and saved in ~/simcode/old-code on my account
% on the mathematics machines.

% Many files need access to these global variables.
% Gridlines sets the mesh refinement; alpha sets the contact
% angle of the film at the boundary. At some point the total
% time for which the solver is run may also become a global,
% for minplot.m's use.

global gridlines alpha
gridlines = 30;
alpha = -2;

% X sets the discrete values of the spatial variable on
% which the ODEs in t are to be solved. Note that we do not
% define X all the way out to the boundaries of the interval
% [0, 1] because of the stencil size.

X = linspace(2/gridlines, 1 - 2/gridlines, gridlines-3);

% Y_0 sets the initial condition. It should be of the
% same length as X.

Y_0 = .1*ones(1, length(X));

% runtime is the total length of time for which we want
% ode15s to solve the system it is given. This may
% eventually become a global.

runtime = .0195;

% Solve the system and output the result as a struct.

sol = ode15s(@filmde, [0 runtime], Y_0);

% Unlike X, above, Xplot does span the entire interval
% [0, 1]. As the name suggests, we use it for plotting
% purposes so that we can see values across the entire domain.
```

```
Xplot = linspace(0, 1, gridlines+1);

% Initializing yvals for use in the for loop below is
% probably not entirely necessary, but it does ensure
% that yvals is the proper size.

yvals = zeros(gridlines + 1);

% Create an array of uniformly spaced timesteps. The last
% argument in linspace determines the size of this array.
% Use your best judgment as to this value; if you make it
% too small, all the interesting things will happen between
% the first two timesteps and it will appear as though only
% the initial and final conditions have been plotted as the
% film converges so quickly to the minimizer. On the other
% hand, if it is too large, the eventual animation of the
% solution will take prohibitively long to display. There is
% nothing, however, preventing you from using a smaller
% value than runtime for the endpoint of consttime.

consttime = linspace(0, runtime, 200);

% Get values of the film height for specific, uniformly
% spaced timesteps.

yeval = deval(sol, consttime);

% The following loops interpolate the values of the film
% height at the boundary where the stencil prevents us from
% doing so with the ODE solver itself, then plots the values
% we got from deval against Xplot. pause(.1) causes it to
% wait .1 sec between frame refreshes; user should be prepared
% either to reduce the index to something smaller than
% length(consttime) or be prepared for the fact that
% the animation will take .1*length(consttime) seconds
% to run after all computations are complete.

for i = 1 : length(consttime)
   for j = 1 : gridlines - 3
```

```
        yvals(j + 2) = yeval(j, i);
    end
    yvals(1) = (12/5)*yvals(3) - (64/35)*yvals(4) + ...
        (3/7)*yvals(5) - (36/35)*alpha/gridlines;
    yvals(2) = 2*yvals(3) - (9/7)*yvals(4) + ...
        (2/7)*yvals(5) - (2/7)*alpha/gridlines;
    yvals(gridlines) = 2*yvals(gridlines-1) - ...
        (9/7)*yvals(gridlines-2) + ...
        (2/7)*yvals(gridlines-3) - ...
        (2/7)*alpha/gridlines;
    yvals(gridlines + 1) = (12/5)*yvals(gridlines-1) - ...
        (64/35)*yvals(gridlines-2) + ...
        (3/7)*yvals(gridlines-3) - ...
        (36/35)*alpha/gridlines;

    pause(.1);
    plot(Xplot, yvals);
end

% Now we plot y = 0 in a different color so that it
% is easier to visually observe that the film has touched
% down and would rupture if the numerical scheme could
% continue solving.

hold on;
plot(Xplot, zeros(1, length(yvals)), 'r-');
hold off;

% This outputs the struct given by the ode15s routine;
% we can make use of this in minplot.m.

solout = sol;
```

A.4 Minimum Plots

The `minplot.m` function is intended as a tool for refinement analysis. It will take as input the `struct` output by an ODE solver, evaluate its values at uniform timesteps, and output the minimum film thickness at each timestep both as an array of values for future data analysis and as a semilog plot for immediate observation of results.

```
function ymins = minplot(y, timetotal)

% MINPLOT
% R.M. Baur
% Originally created: 29 March 2005
% Last Modified: 10 April 2005
% HMC Mathematics Senior Thesis, Spring-Fall 2005

% MINPLOT takes as input the struct output from ode15s.
% It passes it through deval to get values at regular
% timesteps, then finds the minimum film thickness at each
% of these timesteps. It then plots these minima on a log
% scale against time on a linear scale.

% NOTE: As of this writing, the user must input the total
% time for which the ode15s solver was run, so that minplot
% can tell deval how many timesteps to use. Please keep
% track of this when running solver.m so that your data
% from minplot will be accurate.

% Use totalsteps to decide how often you want deval to
% calculate y values.

totalsteps = 2000;

timesteps = linspace(0, timetotal, totalsteps);

yeval = deval(y, timesteps);

minvals = min(yeval);

semilogy(timesteps, minvals);

ymins = minvals;
```

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